# Ab initio calculations of electronic response - ingredients, results and challenges

Lucia Reining, and Palaiseau Theoretical Spectroscopy Group

*Laboratoire des Solides Irradiés, CNRS-Ecole Polytechnique*
*91128 Palaiseau, France*

Today, one of the big challenges of theoretical condensed matter physics is to find ways for describing accurately and efficiently the response of electrons to a perturbation. In fact, spectra such as absorption or electron energy loss can be directly derived from response functions. More indirectly, but as importantly, response functions enter the description of correlation effects, for example the screening of the hole left by the photoelectron in a photoemission experiment.

We will give an overview of the role of the dynamical dielectric screening in various theoretical and experimental situations. We will point out which contributions and effects are dominant for certain materials and certain kinds of spectroscopy. We will summarize the two main lines of development that are today followed in the community of theoretical solid state physics (namely, many-body Green's functions and density-functional based approaches [1,2]). We will discuss the fundamental ideas, possible combinations [3], contributions to the interpretation of experimental results, and limitations.

The various aspects - including the limitations - will be illustrated with results for the plasmon dispersion in carbon nanostructures [4], photoemission spectra of transition metal oxides [5], and energy levels and absorption spectra of complex materials for technological applications, like data storage [6] or solar cells.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).

[2] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002).

[3] F. Bruneval et al., Phys. Rev. Lett. **94**, 186402 (2005).

[4] C. Kramberger et al., Phys Rev. Lett. (in press)

[5] M. Gatti et al., Phys. Rev. Lett. **99**, 266402 (2007)

[6] W. Welnic et al., Phys. Rev. Lett. **98**, 236403 (2007)